

PROGRAMME DAY 3: WEDNESDAY 5 DECEMBER 2018

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07.00 - 09.00	BREAKFAST								
09.00 - 09.45	PLENARY LECTURE: PAULA HAMMOND - MASSACHUSETTS INSTITUTE OF TECHNOLOGY (BENELUXZAAL) DESIGNER POLYPEPTIDES FOR CANCER THERAPEUTICS AND CONTROLLED MRNA DELIVERY								
ROOM	80-81	82-83	PARKZAAL	AUDITORIUM	55-57	58	63-64	65	BOSZAAL
	NEW STRATEGIES TOWARDS USEFUL MOLECULES Chair: Tatí Fernández Ibáñez	MO-BASED CATALYSTS! Chair: Gadi Rothenberg	PHOTOCATALYSIS Chair: Bastian Mei	SELF-ASSEMBLY IN SOFT MATTER Chair: Roxanne Kiełtyka	PROBING NANOSTRUCTURE WITH SPECTROSCOPY Chair: Wybren Jan Buma	OPTO-ELECTRONIC MATERIALS AND SPECTROSCOPY CHAIR: ANDRIES MEIJERINK	DISORDER IN SOFT SOLIDS Chair: Wouter Ellenbroek	SELF-ASSEMBLY & SURFACTANTS Chair: Daniela Kraft	NETWORKS & PARTICLES Chair: Loai Abdelmohsen
09.55 - 10.10	J. Perez (RUG, Harutyunyan) Heteroaromatic enolate trapping promoted by Lewis acids	M. Yu (TU/e, Kosinov) Investigation of the active sites in promoted molybdenum sulfide catalysts	C. van Oversteeg (UU, Ngene) Copper sulfide nanocrystals for photocatalytic applications	J. Movili (UT, Huskens) Modified poly-L-lysine for surface functionalization and biosensing applications	M. Failla (TUD, Siebbeles) High charge mobility in two-dimensional pbs nanosheets probed by ultrafast terahertz spectroscopy	M. Gelvez-Rueda (TUD, Grozema) Effect of the organic cation on 2D organic-inorganic Perovskites	J. Verweij (WUR, Van der Gucht) Simplifying structure: elucidating the network topology of colloidal gels	D. Atkins (TU/e, Voets) Engineering biosynthetic extremozymes for cascade reactions in harsh environments	S. Keller (RU, Wilson) Autonomous enzyme-based hydrogel microparticles
10.10 - 10.25	C. Vis (UU, Bruijninx) Catalysis in Pickering Emulsions	I. Vollmer (TUD, Kapteijn) Activity and coking descriptors for Mo and Fe as active metal for methane conversion to aromatics	F. Oropeza Palacio (TU/e, Hofmann) Role of photoreduced surface states on the photoelectrochemical properties of CuBi2O4	C. Facciotti (WUR, Saggiomo) Beyond C3Ms: C4Ms Cyclodextrin-Based Complex Coacervate Core Micelles	D. Petrova (UvA, Brouwer) Fluorescence measurement of nano-viscosity of liquids confined between rough surfaces	W. Franssen (RU, Kentgens) Dimethylammonium incorporation in lead acetate based MAPbI3 perovskite solar cells	J. Rouwhorst (UvA, Schall) Colloidal gelation as a nonequilibrium continuous phase transition	J. B. ten Hove (WUR, Velders) Thin-film gold-nanoparticle loaded dendritic assemblies	E. Maassen (TU/e, Heuts) Development of reversible network chemistry for UV curable materials
10.25 - 10.40	F. Milocco (RUG, Otten) Mono(formazanate) ferrate(III) catalysts for CO2 conversion into cyclic carbonates	X. Xi (RUG, Heeres) Improved Potassium promoted molybdenum sulfide catalysts for mixed alcohols synthesis from syngas	T. Giousis (RUG, Rudolf) A new synthetic route for the development of 2D germanane	A. Hofman (WUR, Kamperman) Synthesis and self-assembly of well-defined strong anionic/hydrophobic diblock copolymers	Z. Ristanovic (LEI, Orrit) Large linear Stark effect on single molecules of dibenzoterylene in 2,3-dibromonaphthalene	M. Izquierdo (RUG, Havenith) Non-radiative decay paths in optoelectronic materials: a computational study	S. Ciarrella (TU/e, Janssen) Tuning and predicting the fragility in glass-forming vitrimers	F. Tosi (RUG, Wezenberg) Control of self-assembly in water by metal ion coordination	M. Kopec (UT, Vancso) Synthesis of (bio)hybrid materials by surface-initiated SARA ATRP
10.40 - 11.00	COFFEE BREAK								
ROOM	80-81	82-83	PARKZAAL	AUDITORIUM	55-57	58	63-64	65	BOSZAAL
FOCUS SESSIONS	Plasmonics for Chemistry Chair: Andrea Baldi	Biobased building blocks from lignin Chair: Erik Heeres	Main group chemistry for the future Chair: Chris Stootweg	Organised by Holland Chemistry Closing the loop of soft materials usage – Chemical recycling and beyond Chair: Katja Loos	Oil paint degradation: an analytical challenge Chair: Katrien Keune	Organised by KNCV, Computational and Theoretical Chemistry Chair: Celia Fonseca Guerra	Catalysis via design of reactive metal - ligand/support interactions Chair: Jarl Ivar van der Vlugt	Applied chemical research innovations with SME's Chair: Patrick Uiterweerd	Computational Science meets Software Development for Energy Research Chair: Evert Jan Meijer
11.00 - 12.20	1. Suljo Linic (Univ. of Michigan) Photocatalysis on plasmonic metal nanostructures 2. Peter Zijlstra (TU/e) Plasmonic nanoparticles to detect and study single biomolecules 3. Jenny Kontoteta (AMOLF) Deposition of Pt catalytic nanoparticles on Au/TiO2 photoelectrodes using "hot-electron" chemistry	1. Nicholas Westwood (St. Andrews) Lignocellulosic biomass: An inspiration for any chemist 2. Douwe Zijlstra (RUG) Extraction of lignin structures with high potential for valorization 3. Pieter Bruijninx (UU) Lignin, some perspectives on catalysis and analytics	1. Rebecca Melen (Cardiff University) Small Molecule Activation and Catalysis Using p-Block Lewis Acids: A Transition Metal Alternative 2. Simon Aldridge (University of Oxford) Bond activation by group 13 and 14 systems 3. Flip Holtrop (UvA) Steric attraction in frustrated Lewis pair chemistry	1. Georg Gübitz (University of Natural Resources and Life Sciences) Designing enzymes for future material processing 2. Valerie Reid (DSM / NIAGA) NIAGA - a polyester based product design philosophy for circular economy 3. Rudy Folkersma (NHL Stenden) Circular Plastics: Research & Education within NHL Stenden	1. Matthias Alfeld (TUD) Large scale X-ray imaging for historical paintings - Capabilities and recent developments 2. Lambert Baij (UvA) Smart design of model systems to study chemical reactions inside historical and modern paintings 3. Joris Spraket (WUR) Light from Within: Illuminating complex dynamics and mechanics in materials and paints	1. Matthias Bickelhaupt (VU) Introducing KNCV-Computational and Theoretical Chemistry (CTC) 2. Ferdinand Grozema (TUD) Quantum interference effects in charge transfer and molecular conductance 3. Shirin Faraji (RUG) Excited-state processes and quantum effects in biological systems 4. Stephanie van der Lubbe (VU) Secondary Electrostatic Interaction Model for Multiply Hydrogen-Bonded Arrays Revisited	1. Carsten Streb (Univ. Ulm) Polyoxometalate-based composites in sustainable chemistry 2. Marine Desage El-Murr (Strasbourg) Redox dialogue between ligands and metal for unconventional reactivities 3. Ruud Kortlever (TUD) Tuning the selectivity of electrocatalytic CO2 reduction on polycrystalline copper with organic additives	1. Gino van Strijdonck (Hogeschool Zuyd) Chemistry between Zuyd and Chemelot 2. Jan Peter Nap (Hanzehogeschool Groningen) CO2 capture and biomethane production: earthquake-free natural gas from Groningen? 3. Ton Vries (Syncom) How two SME Cooperations in the field of Life Science and Green Chemistry work with Universities of Applied Sciences (Hanze), business models and examples	1. Sandra Luber (Univ. of Zürich) Advanced ab initio simulations for study and design of solar light-driven water splitting 2. Lucas Visscher (VU) Automating computational chemistry workflows: prospects and challenges 3. Monika Dash (UT) The quest for accurate modeling of photo-excitations: a quantum Monte Carlo story
12.20 - 13.00	LUNCH								
13.00 - 14.30	POSTER SESSION (ALL POSTERS DAY 3: CHEMISTRY OF MATERIALS & CHEMICAL CONVERSION)								
ROOM	80-81	82-83	PARKZAAL	AUDITORIUM	55-57	58	63-64	65	BOSZAAL
	HYDROGENATION AND DEHYDROGENATION CHEMISTRY Chair: Danny Broere	CATALYSTS CHARACTERISATION Chair: Irene Groot	LIGHT-INDUCED PROCESSES Chair: Ferdinand Grozema	FUNCTIONAL NANOMATERIALS Chair: Giuseppe Portale	CATALYSIS AND SPECTROSCOPY Chair: Shirin Faraji	THEORETICAL/COMPUTATIONAL CHEMISTRY Chair: Katarina Dolbhoff-Dier	COLLOIDS & EMULSIONS Chair: Thomas Kodger	PHASE TRANSITION IN CHEMISTRY Chair: Boelo Schuur	CATALYTIC SYNTHETIC METHODS Chair: Marc-Etienne Moret
14.30 - 14.45	C. van Slagmaat (UM, De Wildeman) The effect of H2 donors upon the solvent-free hydrogenation of levulinic acid by the shvo catalyst	M. Gambino (UU, Meirer) Poisoning metals interaction with zeolite and matrix in a fluid catalytic cracking catalyst particle	A. Goyal (TU/e, Van der Schoot) Impact of substrate wetting on domain morphology and demixing dynamics of binary fluid mixtures	C. Xia (UU, De Mello Donega) Colloidal copper chalcogenide nanocrystals: a versatile new class of optoelectronic materials	B. Venderbosch (RUG, Tromp) Spectroscopic investigation of the activation of a chromium-pyrrolyl ethene trimerisation catalyst	R. Chandran Puthenkalathil (UvA, Ensing) Mechanism of H2 production by [FeFe] hydrogenase enzyme from first principle molecular dynamics	A. van Silfhout (UU, Ern�) Ferrofluids for magnetic density separation	L. Kollau (TU/e, Tuinier) Quantification of the liquid window of deep eutectic systems	M. Faltracco (VU, Ruijter) Catalytic asymmetric synthesis of diketopiperazines via an Ugi/Tsuji-Trost sequence
14.45 - 15.00	A. Krieger (TUD, Pidko) Homogeneous manganese catalysts for the efficient hydrogenation of esters and ketones	W. Vrijburg (TU/e, Hensen) Promotion of Ni/TiO2 catalysts with Mn in CO2 and CO methanation	R. Tempelaar (Columbia, la Cour Jansen) Rapid singlet fission is driven by vibronic resonance and thermodynamics	S. Gudjonsdottir (TUD, Houtepen) Towards permanent electrochemical doping of porous semiconductors	F. Nattino (LEI, Meyer) Temperature-dependent adsorbate-phonon lifetimes from non-equilibrium molecular dynamics simulations	J.P. Menzel (LEI, Buda) Photoinduced electron transfer into a dye-sensitized TiO2 surface: dynamical and solvent effects	R. Dekker (UvA, Bonn) Emulsion destabilization by squeeze flow	M. Smets (RU, Cuppen) To jump or not to jump that is the questions	K. Naksomboon (UvA, Fernandez-Ibanez) Para-selective C-H olefination of aniline derivatives via pd/s,o-ligand catalysis
15.00 - 15.15	N. Govindarajan (UvA, Meijer) Realistic modeling of homogeneously catalyzed dehydrogenation reactions	N. Krans (UU, Zecevic) In-situ imaging of nanoscale processes in liquid: iron nanoparticle attachment to carbon support	A. Pannwitz (LEI, Bonnet) Light-driven electron transfer across lipophilic phospholipid bilayers with molecular wires	R. Kamarudheen (DIFFER, Baldi) Photothermal vs hot charge carrier effects in plasmon-driven syntheses of nanoparticles	E. Nour Ghassemi (LEI, Kroes) Transferability of the specific reaction parameter functional for H2 + Cu(111) to D2 + Ag(111)	S. Simko (UU, Bulo) Protecting a zeolite catalyst from water: a molecular modeling approach	D. Hayden (UU, Imhof) Fully-biobased highly transparent nanopaper with tunable uv-blocking functionality	A. Wadhawan (UvA, Bolhuis) Unravelling the nucleation of methane hydrates	J. Collet (VU, Orru) Nickel-catalyzed imidoalative cross-coupling towards densely functionalized pyrimidouracils
15.20 - 15.50	KEYNOTE: CRISTINA NEVADO - UNIVERSITY OF ZÜRICH (ROOM 82-83) MECHANISTIC PUZZLES IN METAL CATALYZED REACTIONS		KEYNOTE: TANJA WEIL - MAX PLANCK INSTITUTE FOR POLYMER RESEARCH (AUDITORIUM) RESPONSIVE SUPRAMOLECULAR BIOMATERIALS FOR MEDICINAL APPLICATIONS		KEYNOTE: MARK JOHNSON - YALE UNIVERSITY (ROOM 63-64) INTEGRATING CRYOGENIC ION CHEMISTRY AND SPECTROSCOPY: CAPTURE AND CHARACTERIZATION OF REACTION INTERMEDIATES IN HOMOGENEOUS CATALYSIS				
15.55	POSTER PRIZE AWARDS DAY 3 (KEMPENZAAL)								
16.00	CLOSURE								

LEGEND	
CATALYSIS & PROCESS TECHNOLOGY	MATERIALS SCIENCE
SOFT MATTER	ORGANIC CHEMISTRY & POLYMER CHEMISTRY
THEORY & SPECTROSCOPY	